Phase Diagram of a Superconducting and Antiferromagnetic System with SO(5) Symmetry

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Temperature vs. chemical-potential phase diagrams of an SO(5) model for high-T_c cuprates are calculated by Monte Carlo simulation. There is a *bicritical point* where the second-order antiferromagnetism (AF) and superconductivity transition lines merge tangentially into a first-order line, and *the SO(5) symmetry is achieved*. In an external magnetic field, the AF ordering is first order in the region where the first-order melting line of flux lattice joins in. There is a *tricritical point* on the AF transition line from which the AF ordering becomes second order.

The antiferromagnetism (AF) and superconductivity (SC) exist near to each other in the temperature vs. doping-rate phase diagrams of many high-T_c cuprates. It is understood that in these materials the same electrons can contribute either to AF or to SC depending on the doping rate of holes, or the chemical potential of electrons. It is then natural and important to incorporate these two orders into a single theoretical scheme. Zhang proposed a unified theory based on the SO(5) symmetry of SC and AF [1], in which the three components of a spin, and the real and imaginary part of the SC order parameter compose a five-component superspin; the chemical potential plays the role of a symmetry-breaking field. Studies on the SO(5) model are carried out on the symmetry of quantum operators by Rabello *et al.* [2] and on its relation with the long studied Hubbard and $t - J$ models by Meixner *et al.* and Eder *et al.* [3]. Using the SO(5) model Arovas *et al.* showed that the vortex line can have an AF core [4]. A modified SO(5) vector pseudospin model is proposed and studied by Koyama [5]. A systematic thermodynamic study on the SO(5) model is still lacking, which is important because the entropy effect in this model is significant, and ultimately one should compare the predictions by the model with phase diagrams observed experimentally. To reveal the thermodynamic behavior of the SO(5) model is also of interests from the viewpoint of the theory for phase transitions and critical phenomena. As shown in the following, the high-T_c cuprates may be a new class of materials which show multicriticality, like magnets and liquid crystals.

In this Letter, we report on our Monte Carlo (MC) study of a classic version of the SO(5) model. Our main results are as follows: There are normal (N), AF, SC and phase-separation (PS) phases in the temperature vs. chemical-potential phase diagram. The N-AF and N-SC phase transitions are second order in the 3D Heisenberg and XY universality classes, respectively, while those between the ordered phases are first order. The N-AF and N-SC lines merge tangentially at a *bicritical point* of a finite temperature into the first-order AF-SC line on which the PS-AF and PS-SC lines collapse in the vicinity of the bicritical point. *By checking the weights of the SC and AF components it is confirmed in the present simulation that the SO(5) symmetry is achieved at the bicritical point.* In the presence of an external magnetic field, the N-AF phase transition is first order in the vicinity of the point where the N-AF line meets the first-order melting line of the flux lattice (N-SC line). *There is a tricritical point on the N-AF line from which the phase transition becomes second order. This change in the order of phase transition is originated from the thermal fluctuations enhanced by the SC degrees of freedom, and is an important implication of the SO(5) theory.*

Generally speaking the thermodynamic nature of a phase transition is governed by the symmetry of the degrees of freedom, dimensionality, and range of interactions. Quantum effects are less important as far as the phase transition occurs at a finite temperature. Therefore, in the present study we adopt the following classical SO(5) Hamiltonian on the simple cubic lattice:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \cos\theta_i \cos\theta_j \cos(\varphi_i - \varphi_j) + J \sum_{\langle i,j \rangle} \sin\theta_i \sin\theta_j \mathbf{S}_i \cdot \mathbf{S}_j + g \sum_i \sin^2\theta_i \tag{1}$$

with $J > 0$, $\mathbf{S}_i^2 = 1$. The first term is for the SC order parameters where φ's are the phase variables, reminding that a superconducting transition is expected to belong to the 3D XY universality class. The second term is for the AF components. The parameter g is a renormalized chemical potential [1,4], and a negative g favors AF components.

Hamiltonian (1) is equivalent to the classical version of the SO(5) vector pseudspin model presented in Ref. [5]. At each MC step, a trial configuration of superspins is generated with $\sin^2 \theta = 1/2$ in average and is then subjected to the standard Metropolis prescription under Hamiltonian (1). This process reduces significantly the simulation time for generating symmetric 5-vector superspins where each component should have a weight of $1/5$ in average. The loci of the bicritical and tricritical points in phase diagrams may be shifted somehow to the negative g direction. However, the important features, such as the properties around the bicritical point and the existence of a tritritical point in an external magnetic field, should remain unchanged since they are determined by the symmetry of the Hamiltonian. Periodic boundary conditions are put in all the directions.

The temperature vs. chemical-potential phase diagram is depicted in Fig. 1 using a system of size $L^3 = 40^3$. A bicritical point [7] is observed at $[g_b, T_b] = [-1.04J, 0.845J/k_B]$, where the N-AF and N-SC lines merge tangentially. By checking the weights of the SC and AF components it is confirmed that the SO(5) symmetry is recovered at the bicritical point. The critical temperature for the SC ordering, $T_{XY}(g)$, is higher than that of the AF ordering, $T_N(g)$, for the same value of $|g - g_b|$. These two phase transitions are in the 3D XY and Heisenberg universality classes, respectively, in spite of the existence of the competing degrees of freedom. Singularities in the temperature dependence of the weight $\langle \sin^2 \theta \rangle$ are observed only at the phase boundaries. Therefore, no crossover temperatures such as T_s and T_p in Ref. [1] can be defined. The superspin flips are incomplete even at the phase transitions at finite temperatures in the sense $0 < \langle \sin^2 \theta \rangle < 1$.

The segment between $[g_b, T_b]$ and $[0, 0]$ is considered as the first order SC-AF phase boundary. This first-order phase transition is the counterpart of the spin-flop transition in the uniaxially anisotropic antiferromagnets in a magnetic field parallel to the easy axis, as first pointed out by Néel [6] and investigated by others [7,8]. In the simulations, we observed the following hysteresis behaviors: Heating the system from an AF configuration with $\sin \theta = 1$ at zero temperature, we observe a first-order AF to SC phase transition at $T_{ht}(g)$ when $g_b < g < 0$; Cooling the system in the SC phase, a first-order SC to AF transition occurs at $T_{cl}(g)$ when $g_b < g < -0.6J$, with $T_{cl}(g) < T_{ht}(g)$. In the region $g > -0.6J$, the SC order survives down to zero temperature. This hysteresis phenomenon suggests the coexistence of the SC and AF orders, presumably in the form of phase separation, in the parameter region shown in Fig. 1. The PS phase shrinks as the chemical potential decreases and approaches g_b. Near the bicritical point $[g_b, T_b]$, the $T_{cl}(g)$ and $T_{ht}(g)$ lines collapse into a single line which is tangential to $T_{XY}(g)$ and $T_N(g)$ lines at the bicritical point. Increasing g from g_b, the latent heat associated with $T_{ht}(g)$ increases from zero, assumes its maximum $Q \simeq 0.2J$ at $g \simeq -0.8J$, then decreases and becomes zero at $g = 0$; the one associated with $T_{cl}(g)$ increases linearly from zero to $Q \simeq 0.6J$ at $g \simeq -0.6J$

In order to see the effect of anisotropy in the couplings, we have also simulated the Hamiltonian with $\Gamma^2 = J/J_c^{SC} = 10$ (for the definition of Γ see Hamiltonian (2) in below). The phase diagram is shown in the right inset of Fig. 1 using a system of size $L^3 = 20^3$. $T_{XY}(g)$ becomes lower than $T_N(g)$ for the same value of $|g - g_b|$, as in experimental observations of high-T_c cuprates. The bicritical point is at $[g_b, T_b] = [0.23J, 0.65J/k_B]$ for this anisotropic case.

An external magnetic field will couple with the AF moments in the Zeeman form, and meanwhile modify the phases

of SC order parameters. In an external magnetic field along the c axis ($\hat{c} \parallel \hat{z}$), the Hamiltonian should be

$$\mathcal{H} = -J \left[\sum_{\langle i,j \rangle \parallel ab\text{plane}} \cos\theta_i \cos\theta_j \cos\left(\varphi_i - \varphi_j - \frac{2\pi}{\phi_0} \int_i^j \mathbf{A}^{(2)} \cdot d\mathbf{r}^{(2)}\right) + \frac{1}{\Gamma^2} \sum_{\langle i,j \rangle \parallel c\text{axis}} \cos\theta_i \cos\theta_j \cos(\varphi_i - \varphi_j) \right]$$
$$+ J \sum_{\langle i,j \rangle} \sin\theta_i \sin\theta_j \mathbf{S}_i \cdot \mathbf{S}_j - H \sum_i \sin\theta_i S_{iz} + g \sum_i \sin^2\theta_i. \tag{2}$$

This Hamiltonian can be derived from the Ginzburg-Landau (GL) Lawrence-Doniach (LD) free energy functional [9,10] with the additional AF components. The GL free energy functional was used by Arovas *et al.* [4] to discuss the AF vortex core. In the present study we adopt $f = 1/25$ which means that there is one flux line per 25 unit cells in the ab plane. The system size is $L_x \times L_y \times L_z = 50 \times 50 \times 40$, and there are 100 flux lines induced by the external magnetic field in the system. The anisotropy constant is taken as $\Gamma^2 = 10$. The magnetic induction is evaluated as $B = 10\phi_0/[25(\gamma d)^2]$ for a high-T_c cuprate of the distance between neighboring CuO$_2$ bilayers d and the material-dependent anisotropy constant γ [10]. We have put $H = 0.1$ in the Zeeman term, and confirmed that this field confines the AF components almost perfectly in the ab plane. The value of H is irrelevant to the phase transitions and the phase diagram shown below, till it increases to a critical value to cause the spin-flop transition in the AF components. This aspect will be discussed elsewhere.

The phase diagram for $\Gamma^2 = 10$ is shown in Fig. 2. The N-SC phase transition is the well established, first-order melting of flux-line lattice [11]. Cooling the system across the melting point $T_m(g)$, the helicity modulus sets up sharply from zero; a δ-function peak in the specific heat is detected associated with a tiny latent heat of order of $0.001J$ per site; the flux lines manifest themselves into the Abrikosov lattice; the hysteresis loop associated with this first-order melting is very small. These observations are the same as those in absence of the AF degrees of freedom [10]. The cores of flux lines are of finite AF components in the present case, as discussed by Arovas *et al.* [4].

The effect of the competition between the AF and SC degrees of freedom in the same Hamiltonian is most pronounced in the region around $[g_{\mathrm{x}}, T_{\mathrm{x}}] = [0.56J, 0.41J/k_B]$ where the N-AF line meets the first-order N-SC line. Namely, the N-AF phase transition is first order as seen in Fig. 3 for a cooling process of $g = 0.5J$. Hysteresis behaviors are observed as denoted by $T_{Nht}(g)$ and $T_{Ncl}(g)$ in Fig. 2. The change of the usual second-order AF ordering to first order is because of the big thermal fluctuations enhanced by the SC degrees of freedom in the external magnetic field. There is a tricritical point [12,8] on the N-AF line at $[g_t, T_t] = [0.40J, 0.59J/k_B]$. The temperature dependence of the staggered magnetization and specific heat, as well as the weight of AF components are depicted in Fig. 4 for $g = g_t$. Presuming single power-law singularities and using the data in the critical region $0.490 \leq k_B T/J \leq 0.584$, we obtain the tricritical exponents $\beta = 0.24 \pm 0.02$ for the staggered magnetization and $\alpha' = 0.47 \pm 0.06$ for the specific heat below the tricritical point, and the tricritical point $k_B T_t/J = 0.59 \pm 0.01$. For the specific heat above the tricritical point one clearly has $\alpha = 0$ from Fig. 4. These tricritical exponents are consistent with those in literature [12]. Discussions about the logarithmic corrections to the power-law functions suggested by the renormalization group will be given elsewhere. We notice that *the first-order AF ordering for $g_t < g < g_{\mathrm{x}}$ and the existence of the tricritical point on the N-AF line are important implications of the SO(5) theory*. The AF ordering at $T_N(g)$ switches back to a

second-order transition for $g < g_t$. The phase transition from the normal phase to the Abrikosov SC phase is always first order, reflecting the fact that the SC order parameters in an external magnetic field have symmetry different from a simple 2-vector model. Our simulated phase diagram in Fig. 2 is hence not included in the list of possible phase diagrams by mean-field theory and renormalization group [8].

In summary we have computed the phase diagram of a classical version of Zhang's SO(5) model. We have found a bicritical point at a finite temperature where the second-order AF (3D Heisenberg class) and SC (3D XY class) transition lines merge tangentially into a first-order line. By checking the weights of the SC and AF components, we have observed the SO(5) symmetry at the bicritical point. Phase separation between the AF and SC orders is observed as the first-order line splits into the supercooling and superheating lines. In the external magnetic field along the c axis, we have found a tricritical point on the AF transition line where the phase transition changes from second order into first order for larger chemical potentials. Quantum fluctuations in the AF components of spin $S = 1/2$ are not included in the present calculation which may reduce the bicritical point. A quantum Monte Carlo simulation on the quantum SO(5) model is hence an interesting future problem. In order to compare quantitatively the simulated phase diagrams with the temperature vs. carrier-concentration phase diagrams for high-T_c cuprates, or the temperature vs. pressure phase diagrams for organic superconductors, one should reduce the SC coupling constants from the value of the AF ones.

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Figure Captions

Fig. 1: Temperature vs. chemical-potential phase diagram of the SO(5) model. N: normal phase; AF: antiferro-magnetic ordered phase; SC: superconducting phase; PS: AF and SC phase-separation phase. The mark b denotes the bicritical point. The left inset shows the zoomed-in phase diagram around the bicritical point. The right inset displays the phase diagram for the anisotropic case of $\Gamma^2 = J/J_c^{SC} = 10$.

Fig. 2: Temperature vs. chemical-potential phase diagram of the SO(5) model in an external magnetic field. The mark t denotes the tricritical point. SC denotes the superconducting Abrikosov flux-line-lattice phase. The magnetic field in the Zeeman term is $H = 0.1J$.

Fig. 3: Temperature dependence of the internal energy, specific heat (A); staggered magnetization $\mathbf{m}_{\text{stag}} = \langle \mathbf{S} \sin\theta \rangle_{\text{stag}}$, weight of AF components, and helicity modulus along the c axis (B), for a cooling process of $g = 0.5J$ where a first-order AF ordering is observed. The magnetic field in the Zeeman term is $H = 0.1J$.

Fig. 4: Temperature dependence of the staggered magnetization $\mathbf{m}_{\text{stag}} = \langle \mathbf{S} \sin\theta \rangle_{\text{stag}}$, weight of AF components and specific heat at $g_t = 0.40J$ where the tricriticality is observed. The magnetic field in the Zeeman term is $H = 0.1J$.